



Experimental study of ethylene counterflow diffusion flames perturbed by trace amounts of jet fuel and jet fuel surrogates under incipiently sooting conditions

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ABSTRACT

The structure of an ethylene counterflow diffusion flame doped with 2000 ppm on a molar basis of either jet fuel or two jet fuel surrogates is studied under incipient sooting conditions. The doped flames have identical stoichiometric mixture fractions ($z_f = 0.18$) and strain rates ($a = 92 \text{ s}^{-1}$), resulting in a well-defined and fixed temperature/time history for all of the flames. Gas samples are extracted from the flame with quartz microprobes for subsequent GC/MS analysis. Profiles of critical fuel decomposition products and soot precursors, such as benzene and toluene, are compared.

The data for C7–C12 alkanes are consistent with typical decomposition of large alkanes with both surrogates showing good qualitative agreement with jet fuel in their pyrolysis trends. Olefins are formed as the fuel alkanes decompose, with agreement between the surrogates and jet fuel that improves for small alkenes, probably because of an increase in kinetic pathways which makes the specifics of the alkane structure less important.

Good agreement between jet fuel and the surrogates is found with respect to critical soot precursors such as benzene and toluene. Although the six-component Utah/Yale surrogate performs better than the Aachen surrogate, the latter performs adequately and retains the advantage of simplicity, since it consists of only two components.

The acetylene profiles present a unique multimodal behavior that can be attributed to acetylene's participation in early stages of formation of soot precursors, such as benzene and other large pyrolysis products, as well as in the surface growth of soot particles.

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1. Introduction

Transportation fuels, including jet fuels, constitute a significant share of the world's energy consumption. Common jet fuels include Jet A-1, Jet A, and JP-8. They comprise hundreds of aromatic compounds and aliphatic components, such as straight chain paraffins, branched chain paraffins, cycloparaffins, and alkenes [1]. Depending on the source of the parent crude and the refinery process, their composition may vary significantly. The future fuel supply will become more and more diversified and burning a broad range of fuels as well as reduction of pollutant (e.g., soot) formation will pose new challenges to the implementation of their combustion. This trend will necessitate fundamental studies in well-defined and well-controlled environments to establish, among

other aspects, the chemical kinetic behavior of these complex fuel blends.

Characterization and simulation of jet fuel chemical kinetics and transport is only practical by identifying surrogate mixtures having a relatively small number of components. Colket et al. [2] proposed a road map for future development of surrogate fuels, which resulted from discussions at a number of meetings of a surrogate fuel working group. The surrogate physical and chemical properties should capture essential features of real fuels in prototypical combustion conditions. Surrogate mixtures have been defined and tested in many experimental conditions and configurations, including flow/stirred reactors, shock tubes, premixed flames, pool fires, and counterflow diffusion flames. A comprehensive review was presented by Dagaut et al. [3]. In the late 1980s, Wood et al. [4] formulated a 14-component JP-4 surrogate based on its compound class composition and distillation curves. Subsequent efforts by Schulz et al. [5] led to a 12-component jet fuel surrogate. Feasibility, simplicity, fuel class similarity, and cost are essential criteria that guided subsequent work aimed at decreasing the number of components to produce more manageable formulations. Violi et al. [6] reported a six-component Utah surrogate de-

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signed to match the volatility of jet fuel and its overall sooting behavior based on smoke point tests. More recently, the number of components has further decreased [7–9], with the minimization effort culminating in the two-component Aachen surrogate [10]. Single-component surrogates, though initially contemplated, are now generally thought to lack the necessary flexibility to match the jet fuel performance in a sufficiently broad parameter space. In recent work in pressurized flow reactors, Natelson et al. [11] experimentally studied jet fuel and a three-component jet fuel surrogate suggested by the surrogate fuels working group at pressures as high as 0.8 MPa. The three-component surrogate showed higher reactivity than jet fuel suggesting that an improvement is possible by adding iso-paraffins. Experiments by Holley et al. [12] in a counterflow non-premixed configuration found that the six-component Utah surrogate [6] increased ignition propensity and resistance to extinction compared to jet fuel. This behavior was attributed to mismatched transport properties. Vasu et al. [13] measured ignition delay times of jet fuels in a shock tube and compared them with predictions of some current kinetic mechanisms [14,15]. The five-component Utah surrogate (Violi Surrogate #3 [6]), when used with the Milan mechanism [14], revealed the closest agreement in ignition delay times, especially in capturing the high-temperature trend. This work has continued on individual components of the surrogate mixture, *n*-dodecane ($n\text{-C}_{12}\text{H}_{26}$) and methylcyclohexane (MCH), with shock-tube experiments on the former [16] and with measurements of OH time-histories of oxidation behind reflected shocks for the latter [17].

In our earlier study at Yale [18], good agreement was reported for extinction strain rate and temperature profiles between jet fuel and a six-component surrogate in *non-sooting* counterflow diffusion flames. This contribution began in collaboration with the research groups at University of Utah and University of Milan, with the Utah group establishing the surrogate mixture formulation and the Milan group developing the chemical kinetic model for this surrogate including 221 species and 5032 reactions [18]. The formulation used in [18] and in all subsequent work at Yale departs slightly from the Utah surrogate in that the vol% composition of the six components (Surrogate #1) in Violi et al. [6] was reinterpreted as molar fractions, which resulted in relative average changes of 27% in the component molar compositions. We shall refer to this surrogate, whose composition is specified in Table 1 below, as the Utah/Yale surrogate. More detailed investigations followed in our laboratory, with the chemical analysis of the structure of a methane counterflow diffusion flame perturbed with thousands of ppm of either jet fuel or the six-component jet fuel surrogate [19,20] in highly diluted and *non-sooting* flames, including detailed one-dimensional modeling using the Milan mechanism. The surrogate captured the general jet fuel behavior reasonably well except for ethylene and small aromatics such as benzene and toluene. The discrepancy in aromatics is cause for concern, if confirmed under sooting conditions, since aromatics are critical precursors to soot.

The sooting behavior of jet fuels, especially at take-off, is an issue in most aero-turbines for which non-premixed configurations are preferred. Therefore, any surrogate formulation needs to be validated with respect to this performance. Gas sampling is problematic in the presence of large amounts of soot because of the inevitable clogging of the microprobe orifice. This problem can be circumvented if conditions of *incipient sooting* are chosen, in which the soot loading is kept at the minimum necessary to discern a faint blackbody luminosity in the flame. These are the conditions chosen in the present study.

A comprehensive investigation is conducted on the detailed flame structure of ethylene counterflow diffusion flames perturbed by trace amounts (2000 ppm, molar) of jet fuel and two surrogates via gas sampling and chemical analysis. The ultimate goal is to

ascertain if the surrogate formulations are reasonably successful in mimicking the performance of jet fuel, especially with respect to the behavior of small aromatics for which discrepancies were observed under non-sooting conditions [19,20]. Two surrogates are examined: the six-component Utah/Yale surrogate used in all previous work in our laboratory [18–20], and a two-component Aachen surrogate, that has been reported to mimic not only conditions of extinction and autoignition, but also to match the soot volume fraction behavior, especially under relatively high strain rates [10]. Semi-detailed chemical kinetic mechanisms are available for both surrogates [10,21,22].

2. Experimental setup

Fig. 1 shows a schematic of the experimental setup. It consists of a counter-flow burner [19], including a nitrogen shroud that shields the flame from room drafts and ensures burning in the controlled atmosphere that is determined by the composition of the feed streams. The inner diameter of the fuel and oxidizer outlets is 12.5 mm and the burner separation is 14.1 mm. Slightly nitrogen-diluted air is used as the oxidizer while the fuel is nitrogen-diluted ethylene doped with either jet fuel or the surrogates. To ensure complete vaporization of the dopant liquid, an electro-spray operated in the multi-jet mode [23] disperses the liquid fuel in the preheated fuel/nitrogen stream. This approach provides flexibility in flow rates without compromising the stability of the flame. To prevent condensation downstream of the electro-spray unit, PID controllers keep the fuel line at 430 K, which is well above the dew point of the dopant/ $\text{C}_2\text{H}_4/\text{N}_2$ mixtures. Gas samples are extracted from the flame through a microprobe, consisting of a small silica probe with an outer diameter of 340 μm and an inner diameter of 170 μm . Details of the different microprobes used previously can be found in [19,20].

The chemical analysis is performed by a gas chromatograph (Agilent 6890A) equipped with mass spectrometer (MSD, Agilent 5973N), thermal conductivity (TCD), and flame ionization (FID) detectors. The instrument is capable of quantifying complex hydrocarbon mixtures, CO, CO_2 , O_2 , and N_2 . It uses two capillary columns, a Supelco Carboxen and an Agilent HP-1, connected to the FID and MSD, respectively. In addition, the TCD measures non-hydrocarbon stable gases separated by means of a third column (Alltech, Packed Molecular Sieve). Because of its much wider linear range, this detector is better suited than the MSD for the analysis of gases present as large fractions of the gas sample and/or in greatly varying amounts, e.g., N_2 and O_2 . A homemade nickel-based catalytic converter (Methanizer) allows for FID quantification of CO and CO_2 upon their conversion into methane in the presence of hydrogen. The system can separate and quantify H_2 , N_2 , O_2 , CO, CO_2 , light gaseous hydrocarbons, and higher hydrocarbons up to at least C14.

Species are identified during the GC/MS data post-processing by both the column retention time and the molecule-specific mass spectrum. GC/MS analysis produces a wealth of information, but has one main drawback: it takes a very long time to perform a flame scan. At the small liquid flow rates of interest for jet fuel (e.g., 1.6 ml/h), a syringe pump is used to deliver the fuel. Preserving a steady flame over the analysis time, which is on the order of one day, would be challenging: it would require repeated flame shut-offs for reloading of the syringes. Thermal transients would affect boundary conditions, and other inevitable consequences such as sampling probe distortions might cause reproducibility problems that affect the self-consistency of the data. To sidestep these problems, a semi-automated chemical analysis method is employed that consists of sampling the gas and storing it in a battery of sampling loops using two pneumatic-actuated injection

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